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TECHNICAL NOTE

REPORT FROM THE INTERNATIONAL SUMMER INSTITUTE IN QUANTUM CHEMISTRY AND SOLID STATE PHYSICS HELD AT THE UNIVERSITY OF UPPSALA UPPSALA, SWEDEN

Course, July 29 - August 26, 1962, Uppsala

Symposium, August 27 - September 1, 1962, Rättvik, Dalarna

Quantum Chemistry Group
For Research in Atomic, Molecular and Solid State Theory
Uppsala University, Uppsala, Sweden

Sponsored in part by the
AERONAUTICAL RESEARCH LABORATORY, OAR
THROUGH THE EUROPEAN OFFICE, AEROSPACE RESEARCH,
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TABLE OF CONTENTS

1. INTRODUCTION

The 1962 Summer Institute in Quantum Chemistry and Solid State Physics has been brought to conclusion, and I am hereby submitting a report of the activity.

Altogether, the 1962 institute contained more than 200 hours of lectures, seminars and group activities distributed over five weeks. The formal lectures of the course were divided among some of the senior scientists associated with the Uppsala group, namely Professor Ruben Pauncz (Chemistry Department, Technion, Haifa, Israel), Professor Laurens Jansen (Battelle Memorial Institute, Geneva, Switzerland), Dr. Kimio Ohno (Department of Physics, University of Tokyo, Japan), Dr. Andrew Liehr (Mellon Institute, Pittsburgh, Pa., USA), and Professor Per-Olov Löwdin (University of Uppsala and University of Florida). The following scientists contributed to the institute by giving some advanced lectures: Professor A. John Coleman (Queen's University, Kingston, Ontario, Canada), Professor Bernard Pullman and Dr. Alberte Pullman (Sorbonne, Paris, France), Professor Włodzimierz Kołos (Polish Academy of Sciences, Warsaw), and Dr. Bela A. Lengyel (Hughes Research Lab., Malibu, Calif., USA). The following two members of the Uppsala group assisted in giving seminars and guiding the exercises: Fil. lic. Jean-Louis Calais and Fil. lic. Jan Linderberg. Mr. Calais was also chairman of the practical arrangements. Miss Birgitta Warfvinge was treasurer, and Mrs. Karin Ericson and Mrs. Esther Axene acted as secretaries, whereas Miss Kerstin Rundqvist and Miss Birgitta Welander acted as assisting hostesses and secretaries. Mrs. Karin Löwdin was in charge of the ladies program. A complete list of the staff may be found in section 4.

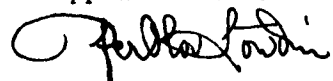
The all-inclusive fee for the course was $ 270 and for all five weeks $ 320; the fee for the symposium alone was $ 75. A sum of $ 4.500 was awarded in stipends from the institute itself to 22 students and scientists from Europe, Asia, and the United States. Thanks to a generous grant from the U.S. National Science Foundation, a sum of $ 5.595 was further made available for the stipends of 11 more American students and scientists.

I would further like to express our most sincere gratitude to the U.S. National Science Foundation and to the OECD organization for their generous support of the organization of the institute. I would also like to thank the permanent sponsors of the Uppsala Quantum Chemistry Group for the indirect support they were giving the institute by supporting the group itself, namely: the Aeronautical Research Laboratory, OAR, through the European Office, Aerospace Research, United States Air Force, the King Gustaf VI Adolf's 70-Years Fund for Swedish Culture, the Knut and Alice Wallenberg's Foundation, the Swedish Natural Science Research Council.

On behalf of the staff, I would like to express our best thanks to the participants for their never-failing enthusiasm and interest and for a most valuable exchange of ideas. Our sincere admiration goes particularly to the experimental chemists and physicists who were so successful in doing theoretical work. It is clear that, with such diverse backgrounds among those present, emphasis had to be placed upon one common field of particular importance, namely the mathematical and conceptual structure of the quantum theory of matter. But even with this limitation, there was enough material for very intense discussions in neighbouring theoretical and experimental fields. The quality of the discussion remarks on the side of the participants tells us that the institute has not failed its purpose.

For us in the Uppsala group, the 1962 institute was a great positive experience, and we hope to be able to repeat this activity again in the summer of 1964.

Uppsala in November 1962



Per-Olov Löwdin
Institute Director

2. ORGANIZATION

The 1962 summer institute in quantum chemistry and solid state physics was the fourth one arranged in Sweden by the Quantum Chemistry Group of the University of Uppsala. As in 1960, the summer institute was arranged in collaboration with the Quantum Theory Project at the University of Florida. The purpose of these institutes is to bring together experimentalists and theoreticians to give them an opportunity to become familiar with recent developments, and to provide a critical survey and summary of methods and theories used in the literature. We have hoped that these institutes would attract scientists from many different countries and research fields for a period of intense collaboration and exchange of ideas, and we feel that these hopes have been fulfilled.

Although the purpose of the summer institutes has been essentially the same in the four cases, the organization has changed slightly, and the courses have been renewed to follow the scientific development. This year, the institute consisted of a four week course in Uppsala followed by a symposium at Rättvik, a little resort town in Dalecarlia. During the course the main emphasis was placed on a careful treatment of fundamental quantum mechanics. This was completed by other lecture series, which dealt more directly with quantum chemical or solid-state topics. - At the symposium there were only invited papers and a great deal of time was devoted to discussions.

The course itself was attended by 78 scientists and, together with the staff, there were more than 100 scientists gathered at the meeting. The daily schedule consisted of 6 formal lectures followed by a question hour. During the latter the main lecturers and part of the junior staff were present, so that the "students" could get obscure points in their notes clarified. These question hours also gave the lecturers the opportunity to find out if the essential points in their presentations were understood. Formal lectures were also given in the evenings during the first week. Exercise sessions were held in the evenings during the remaining part of the course. Parallel with the exercise sessions, a few lectures on selected topics were given.

Detailed programs for the course and the symposium are given in Sec. 3 and Sec. 4, respectively. A summary of the symposium, written by one of the participants, Professor Herbert A. Pohl, is presented in Sec. 5.

It is a pleasure to note that the number of countries represented, shows a marked increase compared to the 1960 institute. Not less than 25 different countries were represented this year. We are happy that our effort in stimulating and catalyzing quantum chemical research has evoked such a response and that these institutes, apart from their possible value for science, may have contributed to international cooperation and goodwill. All lectures and discussions were held in English, which for many participants and some of the staff was a foreign language. Nevertheless, there was no serious language barrier.

Even though the lecture program was heavy, a few outings were arranged including visits to Stockholm, which gave the participants at least some glimpses of Sweden. Some of the participants were quite active in organizing informal social activities in the evenings, and their assistance is gratefully acknowledged.

3. PROGRAM FOR THE COURSE

Survey of weekly schedule

	1st	2nd	3rd	4th	5th week
P.O. Löwdin: Fundamental Quantum Mechanics I	18	14	12	8	
R. Pauncz: Fundamental Quantum Mechanics II	18	10	7	6	
K. Ohno: Molecular Orbital Theory of π-Electron Systems	6	8	4	-	
L. Jansen: Solid State Theory	-	-	6	8	SYMPOSIUM
A. Liehr: Solid State Theory (Ligand field theory)	-	-	6	8	
A.J. Coleman: Density Matrices	-	4	4	-	
A. and B. Pullman: Quantum Theory of Biochemistry	-	-	-	8	
W. Kołos: Numerical Methods in Quantum Chemistry	-	2	4	2	
B. Lengyel: Properties of Hilbert Space.	-	6	-	-	
	42	44	43	40	

Löwdin

Fundamental Quantum Mechanics I

Introduction

I-II. Historical development of quantum theory.

Basic concepts

1. Schrödinger equation.

2. Expectation values and adjoint operators; normal operators; variation principle.

3. Eigenvalue problem; width of an operator; uncertainty relations.

4. Heisenberg's equation and constants of motion.

5. Properties of normal operators; simultaneous eigenfunctions.

6. Normal constants of motion; projection operators.

7. Symmetry of 2-electron systems: $P_{12}H = HP_{12}$; Exchange.

8-9. Antisymmetry requirement and spin; properties of permutations; simple spin functions.

10-11. Exchange phenomenon; Dirac-Van Vleck vector model.

Projection operators and simple symmetry properties

12-13. Projection operators in product form; resolution of identity; cyclic symmetry.

14-17. Translational symmetry for a crystal treated by projection technique: space of reduced wave vector; Bloch projections; Brillouin zones.

Many-particle theory, density matrices, and Hartree-Fock scheme

18-20. Density matrices.

21-22. Natural spin-orbitals.

23-25. Hartree-Fock scheme.

26-28. ASP-MO-LCAO-SCF method.

Hydrogen bonds

29-30. Hydrogen bonds in biochemistry; structure of DNA-molecule.

Time-dependent perturbation theory and irreversible quantum mechanics

31-35. Transition probabilities.

36-37. Irreversibility problem.

Partitioning technique and time-independent perturbation theory

38-40. Partitioning technique and perturbation theory.

41. Reaction operator formalism.

42. Connection with infinite-order perturbation theory.

43-44. Brueckner approximation and modern self-consistent field theories.

Some special problems

45-46. Pauling's electro-negativity concept and many-electron theory.

47-50. Spin interactions: Spin-orbit couplings and Fermi contact terms.

Pauncz

Fundamental Quantum Mechanics II

Mathematical introduction

I-III. Matrix algebra.

IV-VI. Iteration procedures.

Basic concepts: Expansion method and secular equation

1. Expansion theorems; Hilbert space.

2. Completeness concept.

3. Schrödinger equation.

4. Linear system of equations; secular equation.

5-7. Non-orthogonality problem and orthogonalization procedures.

8. Examples of complete sets.

9. Scaling procedure and virial theorem.

10. Expansion of total wave function in terms of Hartree-products and Slater determinants.

11-12. Matrix elements between Slater determinants.

13. Projection splitting of secular equation.

Angular momenta treated by projection operators

14-17. General theory.

18. Orbital angular momenta; spin.

19-22. Applications to atoms; LS-, jj- and intermediate coupling.

Localization of eigenvalues, excited states

23-24. Upper and lower bounds for eigenvalues.

25-26. Variation theorem for excited states.

Relativistic theory

27-29. Dirac equation.

Different orbitals for different spins

30-32. Alternant molecular orbital method.

33-35. Applications to conjugated systems.

Ohno

Molecular Orbital Theory of π-Electron Systems

Basic ideas

1. Hybridization.
2. Basic approximations.
3. Total wave function and use of symmetry.
4. σ-π separation, lone pairs.

Hückel method

5. Defining approximations.
6. Hetero-cyclic molecule, choice of α's.
7. Hetero-cyclic molecules, choice of β's.
8. Charge density and bond order.
9. Alternant hydrocarbons.

ASP-LCAO-MO method

10. Energy calculations.
11. Molecular integrals.
12. Results of calculations on C_2H_4.

13-14. Moffitt's explanation for the failure.

15-16. Pariser-Parr-Pople's semiempirical method.

17. Justification of the scheme.
18. The validity of σ-π separation.

Jansen

Elements of Solid State Theory

Chapter I. Background of the Periodic Potential Problem

1. Introduction.

2. The Hartree-Fock Equations.

3. The One-dimensional Periodic Potential Problem.

Chapter II. The Interesting Electron States in Solids. Review of Existing Methods.

4. The Interesting Electron States.

5-8. Approximate Solutions to the Hartree-Fock Equations.

- A. Crystal Valence Bond Methods.
- B. Crystal Potential Methods.
- C. Purely Variational Methods.
- D. Semi-empirical Approximations.

Chapter III. Group-Theoretical Considerations.

9. Introduction.
Symmetry.
Degeneracy.

10. Some Coset-theorems.

11. Construction of Bases for Irreducible Representations.

12. Space-group Operators.
Substitutional Operators and Space-groups.

13. Irreducible Representations of Space-Groups.

14. Example: The Square Lattice.
Compatibility Relations between Irreducible Representations.

Liehr

Solid State Theory (Ligand Field Theory)

1. Survey of Ligand Field Applications.
2. Ionic Radii.
3. Colors of the $d^{1,9}$ Compounds.
4-5. Colors of the $d^{2,8}$ Compounds.
5-6. Colors of the $d^{3,7}$ Compounds.
7-8. Geometrical Stability of Octahedral Compounds (I).
9. Geometrical Stability of Tetrahedral Compounds (I).
10. Geometrical Stability of Octahedral and Tetrahedral Compounds (II).
11. Geometrical Stability of Octahedral and Tetrahedral Compounds (III).
12-13. Color Depth and Transition Probabilities.
13-14. Comparison of the Ligand Field, Molecular Orbital, and Valence Bond Techniques. Summary.

Program for Summer Institute in Quantum Chemistry and Solid State Physics at Uppsala University

	July 30	July 31	August 1	August 2	August 3	August 4	August 5	August 6	August 7	August 8	August 9	August 10	August 11	August 12
	Monday	Tuesday	Wednesday	Thursday	Friday	Saturday	Sunday	Monday	Tuesday	Wednesday	Thursday	Friday	Saturday	Sunday
9.00 - 9.50	L I	L1	L7	L9	L13	L15		O7	L19	L23	P17	O13	L29	
10.00 - 10.50	LII	L2	L8	L10	L14	L16		O8	L20	L24	P18	O14	L30	
10.50 - 11.20														
11.20 - 12.05	P 1	P3	P5	P7	P9	P11		P13	P15	L25	O11	P21	Ly5	
12.15 - 13.00	P 2	P4	P6	P8	P10	P12		P14	P16	L26	O12	P22	Ly6	
13.00 - 15.00														
15.00 - 15.50	O 1	L3	O3	L11	O5			L17	L21	O9	P19	L27		
16.00 - 16.50	O 2	L4	O4	L12	O6			L18	L22	O10	P20	L28		
17.00 - 17.45	Q	Q	Q	Q	Q			Q	Q	Q	Q	Q		
19.30 - 21.00	Banquet	L5	PI	PIII	PV			Ly1	C1	K1	Ly3	C3		
		L6	PII	PIV	PVI			Ly2	C2	K2	Ly4	C4		

Sight-seeing tour to Stockholm

Crayfish party

parallel with exercises X

Q = Question hour

L = Löwdin P = Pauncz O = Ohno

C = Coleman Ly = Lengyel K = Kolos

J = Jansen Pu = Pullman Li = Liehr

	August 13	August 14	August 15	August 16	August 17	August 18	August 19	August 20	August 21	August 22	August 23	August 24	August 25
	Monday	Tuesday	Wednesday	Thursday	Friday	Saturday	Sunday	Monday	Tuesday	Wednesday	Thursday	Friday	Saturday
9.00 - 9.50	L31	L33	L35	L37	L39	L41		L43	Pu1	L45	Pu5	L47	L49
10.00 - 10.50	L32	L34	L36	L38	L40	L42		L44	Pu2	L46	Pu6	L48	L50
10.50 - 11.20													
11.20 - 12.05	P23	J1	P25	J3	P27	J5	Boat trip to Skokloster	P30	Li9	P32	Li13	Pu7	P34
12.15 - 13.00	P24	J2	P26	J4	P28	J6		P31	Li10	P33	Li14	Pu8	P35
13.00 - 15.00													
15.00 - 15.50	O15	Li1	O17	Li3	Li5			J7	J9	Pu3	J11	J13	
16.00 - 16.50	O16	Li2	O18	Li4	Li6			J8	J10	Pu4	J12	J14	
17.00 - 17.45	Q	Q	Q	Q	Q			Q	Q	Q	Q	Q	
19.30 - 21.00	C5 C6	C7 C8	K3 K4	K5 K6	P29			Li7 Li8	K7 K8	Li11 Li12		Banquet	
	parallel with exercises X							parallel with exercises X					

Due to lack of time a few question hours were used for lectures.

4. PROGRAM FOR THE SYMPOSIUM

Daily schedule: 9 - 10.45, 11.15 - 13.00
Luncheon 13.00
15.00 - 18.00 or 19.00 - 22.00 (depending on weather)

M = Morning
A = Afternoon
E = Evening

MONDAY

Chairman: S.J. Czyzak

M1 Electronic structure of atoms

Watson: Things are worse than you think they are! Comments on the Hartree-Fock theory of atoms. (45 min.)

Kołos: Review of some SCF-CI calculations. (30 min.)

Discussion. (30 min.)

M2 Statistical theory of atoms and molecules

Gáspár: Universal functions in statistical theory. (45 min.)

M3 General discussion of atomic theory

Cusachs: Empirical atomic orbitals. (15 min.)

Discussion: Light atoms, heavy atoms, correlation effects, hyperfine splitting etc. (45 min.)

Chairman: S. Baldursson

A1 Molecular structure (small molecules)

Kołos: The hydrogen molecule treated as a four-body problem. (45 min.)

Moskowitz: Calculation of molecular integrals. (20 min.)

Hoffman: Hückel calculations for polyhedric boron compounds.

A2 General discussion of molecular structure

Electronic and nuclear motion, spectra, spin-orbit coupling etc. (90 min.)

TUESDAY

Chairman: A.J. Coleman

M1 Density matrices in many-body theory

Coleman: Structure of density matrices. (45 min.)

Löwdin: Symmetry properties of natural orbitals. (15 min.)

M2 General discussion of density matrices (45 min.)

M3 Localization of energy eigenvalues

Fox: Survey of methods for finding lower bounds of eigenvalues. (45 min.)

Bazley: Existence and estimation of eigenvalues for the molecular Schrödinger equation. (45 min.)

Discussion. (15 min.)

Chairman: J.M. Wilson

A1 Intermolecular forces

Linderberg: van der Waals forces in non-polar crystals. (30 min.)

A2 General discussion

Chemical reactivity. (50 min.)

A3 Phase problem in theory and experiments

Hedberg: Theory and experiment in gaseous electron diffraction. (30 min.)

E1 Looyenga: Hückel theory without wave functions. (60 min.)

WEDNESDAY

Chairman: R. Pauncz

M1 Correlation problem and symmetry properties; different orbitals for different spin

Pauncz (30 min.)

Dermit: Alternant orbitals in diamond. (45 min.)

Moskowitz: Alternant molecular orbitals for a ring of six hydrogen atoms. (30 min.)

M2 Symmetry properties in Hartree-Fock scheme and in exact theory; general discussion. (105 min.)

Chairman: M. Tomášek

A1 Perturbation theory and reaction operators

Sack: Rayleigh-Schrödinger perturbation expansions to arbitrary order. (45 min.)

Löwdin: Remark on linked-cluster expansion. (15 min.)

Discussion. (30 min.)

A2 Methods for solving the Schrödinger equation; general discussion

Steiner: A perturbation treatment of molecules based on the united atom. (15 min.)

Discussion. (75 min.)

Chairman: P.O. Löwdin

E1 General discussion

Future of Quantum Chemistry. (240 min.)

THURSDAY

Chairman: B. Pullman

M1 Quantum biology; general theory

Pullman: Electronic delocalization and the processes of life. (45 min.)

Discussion. (15 min.)

M2 General properties of DNA and cell control mechanism (105 min.)

Chairman: K. Hedberg

E1 Properties of hydrogen bonds in general; discussion. (60 min.)

E2 Woźnicki: The free-electron model for conjugated systems. (30 min.)

E3 Coleman: The importance of nilpotent operators. (60 min.)

M2 Symmetry properties in Hartree-Fock scheme and in exact theory; general discussion. (105 min.)

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E2 Woźnicki: The free-electron model for conjugated systems. (30 min.)

E3 Coleman: The importance of nilpotent operators. (60 min.)

FRIDAY

Chairman: R.E. Watson

M1 Solid-state theory

Hedin: The theoretical foundation of the one-electron approximation.(45 min.)

Lehman: Calculation of first-order density matrix under the presence of a local perturbation. (45 min.)

M2 Liehr: Geometrical stability of regular polygonal and non-regular polyhedral compounds in degenerate electronic states with small spin-orbit forces. (45 min.)

M3 General discussion of solid-state problems, cohesive properties, etc. (45 min.)

Chairman: D.D. Konowalow

A1 Conductivity problems in solids

Pohl: Electronic processes in molecular solids. (45 min.)

Discussion. (75 min.)

A2 Magnetic properties of solids; exchange problem

Zijlstra: Crystal field effects on magnetic properties of alloys. (30 min.)

Discussion. (30 min.)

SATURDAY

Chairman: R. Pauncz

M1 Current situation in quantum chemistry and solid-state physics

Panel Meeting. (100 min.)

5. SUMMARY OF THE SYMPOSIUM

The Uppsala-Rättvik Symposium on Quantum Chemistry and Solid State Physics, August 1962

Like the ever-widening ripples from a pebble dropped into a pond, the clarifying concepts of quantum mechanics spread wider through the years into all problems of science and life. This was particularly evident at the recent conference sponsored by the Quantum Chemistry Institute at Uppsala University and held at the tiny Swedish resort town of Rättvik in picturesque Dalecarlia, August 27 through September 1st. The Quantum Chemistry Institute, with the stimulating guidance of Professor Per-Olov Löwdin, specializes in attacking those problems in chemistry and solid state physics which may be formulated at the outset in terms of the Schrödinger equation.

The Symposium dealt with a wide range of problems, ranging from the four-body problem for the H_2 molecules, considerations of density matrices in many-body theory, solid state theory and ligand field theory, to recent work in "quantum biology", including suggestive considerations of protonic tunnelling as affecting gene, DNA, RNA, and protein synthesis.

It was clearly apparent in the discussions that the means of application, and even to some extent quantum theory itself in its furthest details and in its time dependency is still under test. Much of the effort reported upon at the Symposium dealt with the means available now to circumvent the considerable mathematical and computational difficulties which beset the quantum chemist. Dr. W. Kołos, of the Institute for Nuclear Research, Polish Academy of Science, Warsaw, described a successful and precise calculation of the H_2 molecule as a four-body problem, including nuclear motion and involving 80 terms. This was regarded by many attending as something of a mile-marker in testing and applying quantum theory.

Headway in attacking problems with the Schrödinger equation was disclo disclosed on several fronts. Profs. A.J. Coleman, P.O. Löwdin, and Dr. Fukashi Sasaki described advances in the density matrix approach and associated boundary value problems in many-body theory, whereas Profs. Norman Bazley and David W. Fox gave new methods for determining lower bounds to the energy levels of atomic and molecular systems. The electron-electron interaction (correlation) problem was also discussed in terms of the alternant molecular orbital scheme (different orbitals for different spins) by Dr. R. Pauncz for hydrocarbons, by Dr. George Dermit for

diamond, and by Dr. J.W. Moskowitz for the interesting hypothetical molecule, annular H_6.

A statistical theoretical study along the lines of the Fermi-Thomas approach was described for atoms by Dr. Rezsö Gáspár. The evaluation of zeta function expansions for molecular integrals was described by Moskowitz. Remarks on linked-cluster expansions were presented by Löwdin. An interesting application of density matrix theory in a Hückel-type approximation was made and applied to conjugated hydrocarbons and benzenoid hydrocarbons containing heteroatoms, by Dr. H. Looyenga, of T.N.O., Delft, Holland.

On hearing the grave and complex computational difficulties facing present day quantum chemists, and of their need to deal with high order determinants, and secular equations where the elements are complex integrals, etc., one is repeatedly struck with the hope that a way out will be found. Perhaps, it will be analogous to the invention of non-unit numerators for fractions which so greatly eased the problems faced by early Egyptians who had conceived only the use of sums of fractions of numerator 1 to express a given fractional value.

Professors Bernard and Alberte Pullman, in masterful presentations, described the considerable progress made in accounting for the relative reactivity and natural selection of many molecules of biological importance. Particular success has been had in the interpretation of the role of enzyme constituents important in redox reactions, in calculating stability to ultraviolet radiation, in evaluating the role of functional molecular portions (as opposed to whole molecules) in carcinogen action, and in the evaluation of hydrogen bonding through the amino acid residues as potential pathways for electron transfer. Löwdin presented an interesting and potentially fruitful notion of protonic tunnelling between the doubly hydrogen-bonded base pairs of the double-stranded DNA molecule. If such a process did occur, it was pointed out, then inversion of pairing and other information mis-storage could occur. This then has direct implication in the problems of mutations, evolution, ageing, and tumor inception.

Remembrance was given the perennial problem of phase determination in electron and X-ray diffraction determinations by Professor K. Hedberg.

New areas for quantum chemistry considerations were seen in (1) the discussion by Dr. Roald Hoffmann of the many new polyhedric organic and inorganic molecules of cage-like structure; (2) in the development by Jan Linderberg of the Nozières-Pines many-electron approach to the treatment of

the dielectric constant of a solid and the consequent estimation of London inter-molecular force terms; (3) in the discussion by Prof. H.A. Pohl of (a) the nature of carrier transport vis-a-vis molecular overlap in molecular solids with special reference to conductivity and to piezo-resistivity, (b) the existing gap in the theory of carrier mobility in solids in the transition range between that well described by wave packet "drifting", and that describable by "hopping" processes (i.e. between about 500 and 0.01 cm^2/ /volt sec.), (c) the much needed extension of theory using random coordinate spacings to the problem of electronic transport processes in amorphous solids and liquids, (d) the problem of the near identity of the activation energy of conduction to the lowest triplet energy in molecular solids of organic nature; (4) Coleman's laudatory reference to the equation of Wentzel for many particles which is relativistically invariant; (5) Löwdin's challenging discussion of the reaction rate problem in terms of the wave mechanical evolution operator for the time dependent Schrödinger equation. Löwdin urged a fresh consideration of the evolution operator in treating kinetic problems and expressed confidence that it would become a powerful tool.

The attending scientists, from many nations, united in expressing their deep appreciation for the hospitality extended them by their Swedish hosts, and for the stimulating approaches in quantum chemistry presented at the Symposium.

Herbert A. Pohl

6. LIST OF PARTICIPANTS AND STAFF

I = Introductory course
S = Symposium
1) = NSF-stipend
2) = OECD-stipend
3) = Institute stipend
* = U.S. citizen

NAME	COURSE	
Aasa, Roland	I	Institute of Physics, Uppsala, Sweden
Ali, Asgar 3)	S	Chemistry Department, Presidency College, Calcutta 12, India
Almgren, Mats	I	Dept of Physical Chemistry, Chalmers Institute of Technology, Gothenburg, Sweden
Arnstein, Rodolphe 3)	I	Service de Chimie-Physique II, Université Libre de Bruxelles, Brussels, Belgium
Ashcroft, Neil William 3)	I	The Cavendish Laboratory, Cambridge, England
Baldursson, Steingrimur 2)	IS	Dept of Chemistry, Háskóli Islands, Reykjavik, Iceland
Banyard, Kenneth E.	IS	Dept of Physics, The University of Leicester, Leicester, England
Bazley, Norman William *	S	Institut Battelle, Carouge-Geneva, Switzerland
Bergson, Göran	S	Dept of Chemistry, University of Uppsala
Burnelle, Louis	IS	Institut d'Astrophysique, Cointe-Sclessin, Belgium
Burns, George *	I	Dept of Chemistry, University of Toronto, Toronto 5, Ontario, Canada
Carnam, Daryl Ann 1) *	S	Quantum Theory Project, Department of Chemistry, University of Florida, Gainesville, Florida, USA
Cooper, Ian Laird	I	Dept of Chemistry, University of Edinburgh, Edinburgh 9, Scotland
Cusachs, Louis Chopin 3) *	IS	Chemistry Dept, Tulane University, New Orleans, La., USA
Czyzak, Stanley J. *	IS	General Physics Research Laboratory (ARP), Aeronautical Research Labs., Wright-Patterson AF Base, Ohio, USA

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